

Interplay of Orbital and Relativistic Effects in Bismuth Oxyhalides: BiOF, BiOCl, BiOBr and BiOI

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Table 1: Calculated lattice parameters and bond lengths of BiOF, BiOCl, BiOBr, and BiOI using the HSE06 with and without Grimme’s D3 dispersion correction. All lattice parameters and bond lengths are given in Å and Volumes are given in Å³. All cell angles were found to be 90°.

BiOF	Experiment	HSE06	HSE+D3
<i>a</i>	3.76	3.74	3.72
<i>c</i>	6.23	6.23	6.20
Volume	87.95	87.01	85.72
Bi–O	2.28	2.27	2.26
Bi–F	2.80	2.78	2.77
BiOCl	Experiment	HSE06	HSE+D3
<i>a</i>	3.89	3.87	3.87
<i>c</i>	7.35	7.95	7.42
Volume	111.11	119.10	110.93
Bi–O	2.32	2.31	2.31
Bi–Cl	3.06	3.06	3.04
BiOBr	Experiment	HSE06	HSE+D3
<i>a</i>	3.92	3.91	3.90
<i>c</i>	8.11	9.23	8.14
Volume	124.75	141.15	124.15
Bi–O	2.33	2.32	2.31
Bi–Cl	3.17	3.20	3.16
BiOI	Experiment	HSE06	HSE+D3
<i>a</i>	4.00	3.99	3.98
<i>c</i>	9.15	10.31	9.15
Volume	146.05	163.97	145.12
Bi–O	2.34	2.34	2.33
Bi–I	3.36	3.38	3.36